Thermodynamics of antiferromagnetic alternating spin chains

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Abstract

We consider integrable quantum spin chains with alternating spins (S_1, S_2). We derive a finite set of non-linear integral equations for the thermodynamics of these models by use of the quantum transfer matrix approach. Numerical solutions of the integral equations are provided for quantities like specific heat, magnetic susceptibility and in the case $S_1 = S_2$ for the thermal Drude weight. At low temperatures one class of models shows finite magnetization and the other class presents antiferromagnetic behaviour. The thermal Drude weight behaves linearly on T at low temperatures and is proportional to the

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central charge c of the system. Quite generally, we observe residual entropy for $S_1 \neq S_2$.

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1 Introduction

Integrable quantum systems and their associated classical vertex models have been extensively studied in the last decades [1, 2]. A large part of these systems is exactly solvable by Bethe ansatz techniques providing spectral data and in some cases also the eigenvectors.

After establishing the integrability and deriving the exact solution for the spectrum, the main questions one likes to answer concern the physical properties of the system in dependence on temperature, magnetic field etc. There are many investigations of integrable system in the thermodynamical limit at finite temperature. In fact, we have several established routes to this goal. One may minimize the free energy functional in the combinatorial Thermodynamical Bethe Ansatz approach (TBA) [3, 4, 5], or one may apply algebraic and analytical means for the computation of the partition function from the quantum transfer matrix (QTM) [6, 7].

The TBA approach is based on the string hypothesis and yields an infinite set of non-linear integral equations (NLIE). However, it is impractical to solve the TBA equations numerically due to the infinite number of equations and unknowns. Therefore approximations are required in this approach.

By means of the quantum transfer matrix approach, a finite set of NLIE can be derived exploiting analyticity properties of the quantum transfer matrix. These equations have been shown to be successful in the description of thermodynamical properties in the complete temperature range for many important models, like the Heisenberg model [7, 8, 9] and its spin-S generalization [10], the $t-J$ model [11], the Hubbard model [12] and $SU(N)$ invariant models for $N \leq 4$ [13].

Nevertheless, the standard construction of the quantum transfer matrix assumes models with isomorphic auxiliary and quantum spaces. Here we are concerned with extensions to more general models with non-isomorphic auxiliary and quantum spaces. Important examples of such systems are mixed spin chains. These mixed chains have been extensively studied for low and high temperatures by use of the TBA equations and finite size scaling for isotropic chains [14, 15]. The dependence on magnetic fields was studied [16, 17, 18, 19] and more recently, also the anisotropic generalization was considered [20].

Our aim is to propose a construction of the quantum transfer matrix by replacing the standard "rotation" of vertex configurations of Boltzmann weights by conjugated representations, i.e. by the normal Boltzmann weight shifted by the crossing parameter. Having this in mind, we can tackle the more general situation where the auxiliary and quantum spaces are not isomorphic. As an application of this idea, we study the generic (S_1, S_2) case of alternating spin chains at finite temperature.

The paper is organized as follows. In section 2, we outline the basic ingredients of the quantum transfer matrix approach. In section 3, we define the alternating spin chain and its properties. In section 4, we derive the set of non-linear integral equations. In section 5, we present our numerical findings for the solution of the NLIE. Section 6 is devoted to the calculation of the thermal Drude weight for the case $S_1 = S_2$. Our conclusions are given in section 7.

2 Quantum transfer matrix

We are interested in the computation of the partition function $Z = \mathrm{Tr}\, e^{-\beta\mathcal{H}}$ in the thermodynamical limit, on the condition that $\mathcal{H}$ is an integrable local Hamiltonian derived from some row-to-row transfer matrix.

In general, transfer matrices can be constructed as ordered products of many different local Boltzmann weights $\mathcal{L}_{\mathcal{A}i}(\lambda)$, where λ denotes the spectral parameter. These weights can be considered as matrices on the space $\mathcal{A}$, usually called auxiliary space, which is related to the degrees of freedom on the horizontal lines of a two dimensional vertex model. The matrix elements of $\mathcal{L}_{\mathcal{A}i}(\lambda)$ are operators acting non-trivially on the site i of the quantum space $\prod_{i=1}^{L} V_i$ of a chain of length L and are related to the degrees of freedom on vertical lines.

The product of Boltzmann weights

$$\mathcal{T}_{\mathcal{A}}(\lambda) = \mathcal{L}_{\mathcal{A}L}(\lambda)\mathcal{L}_{\mathcal{A}L-1}(\lambda)\dots\mathcal{L}_{\mathcal{A}1}(\lambda), \tag{1}$$

defines the monodromy matrix $\mathcal{T}_{\mathcal{A}}(\lambda)$. Here we allowed for non-isomorphic spaces V_i. This way, $\mathcal{L}_{\mathcal{A}i}(\lambda)$ – also called $\mathcal{L}$-operators– may have different representations for the L many quantum spaces $\mathcal{L}_{\mathcal{A}i}(\lambda) = \mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\lambda)$. The labels for different representations, α, β_i, may take for instance integer values $\alpha, \beta_i = 0, \dots, L-1$ and $\mathcal{L}_{\mathcal{A}i}^{(\alpha,\alpha)}(\lambda)$ denotes the isomorphic representation. Then the row-to-row transfer matrix is the trace over the auxiliary space of the monodromy matrix,

$$T(\lambda) = \mathrm{Tr}_{\mathcal{A}}\left[\mathcal{T}_{\mathcal{A}}(\lambda)\right]. \tag{2}$$

The transfer matrix constitutes a family of commuting operators $[T(\lambda), T(\mu)] = 0$, provided there is an invertible R-matrix acting on the tensor product

$\mathcal{A} \otimes \mathcal{A}$, such that

$$R^{(\alpha)}(\lambda-\mu)\mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\lambda) \otimes \mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\mu) = \mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\mu) \otimes \mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\lambda)R^{(\alpha)}(\lambda-\mu). \quad (3)$$

In order to have an associative algebra, the R-matrix is required to satisfy the Yang-Baxter equation

$$R_{12}^{(\alpha)}(\lambda)R_{23}^{(\alpha)}(\lambda+\mu)R_{12}^{(\alpha)}(\mu) = R_{23}^{(\alpha)}(\mu)R_{12}^{(\alpha)}(\lambda+\mu)R_{23}^{(\alpha)}(\lambda). \quad (4)$$

The simplest solution of (3) occurs when auxiliary and quantum spaces V_i are isomorphic implying that $\mathcal{L}_{12}^{(\alpha,\alpha)}(\lambda) = P_{12}R_{12}^{(\alpha)}(\lambda)$, where P_{12} is the permutation operator.

The conserved charges are obtained through the derivatives of the logarithm of the transfer matrix

$$\mathcal{J}^{(n)} = \frac{\partial^n}{\partial\lambda^n} \ln\left[T(\lambda)\right]\Big|_{\lambda=0}, \quad (5)$$

and the Hamiltonian corresponds to the first derivative, $\mathcal{H} = \mathcal{J}^{(1)}$. Therefore, we can relate the transfer matrix and the Hamiltonian in the following way

$$T(\lambda) = T(0)e^{\lambda\mathcal{H}+O(\lambda^2)}, \quad (6)$$

where $T(0)$ plays the role of a kind of right multiple-step shift operator [14] for a general distribution of $\mathcal{L}$-operators $\mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\lambda)$.

Let us consider that in addition to relation (3) the $\mathcal{L}$-operators satisfy the following symmetry properties

$$\text{Unitarity: } \mathcal{L}_{12}^{(\alpha,\beta)}(\lambda)\mathcal{L}_{12}^{(\alpha,\beta)}(-\lambda) = \zeta_{\alpha,\beta}(\lambda)\mathrm{Id}_1 \otimes \mathrm{Id}_2, \quad (7)$$

$$\text{Time reversal: } \mathcal{L}_{12}^{(\alpha,\beta)}(\lambda)^{t_1} = \mathcal{L}_{12}^{(\alpha,\beta)}(\lambda)^{t_2}, \quad (8)$$

$$\text{Crossing: } \mathcal{L}_{12}^{(\alpha,\beta)}(\lambda) = \varsigma_{\alpha,\beta}(\lambda)M_1\mathcal{L}_{12}^{(\alpha,\beta)}(-\lambda-\rho)^{t_2}M_1^{-1}, \quad (9)$$

where $\zeta_{\alpha,\beta}(\lambda)$ and $\varsigma_{\alpha,\beta}(\lambda)$ are scalar functions and ρ is the crossing parameter. Here Id_i and t_i denote the identity matrix and transposition on the i-th space, $M_1 = M \otimes \mathrm{Id}_2$ where M is some scalar matrix.

Now, we can define an adjoint transfer matrix $\overline{T}(\lambda)$ as follows

$$\overline{T}(\lambda) = \prod_{i=1}^{L} \varsigma_{\alpha,\beta_i}(\lambda)\, \mathrm{Tr}_{\mathcal{A}} \left[\mathcal{L}_{\mathcal{A}L}^{(\alpha,\beta_L)}(-\lambda-\rho) \mathcal{L}_{\mathcal{A}L-1}^{(\alpha,\beta_{L-1})}(-\lambda-\rho) \dots \mathcal{L}_{\mathcal{A}1}^{(\alpha,\beta_1)}(-\lambda-\rho) \right], \tag{10}$$

and by using the properties (8-9) we can rewrite the transfer matrix $\overline{T}(\lambda)$ such that,

$$\overline{T}(\lambda) = \mathrm{Tr}_{\mathcal{A}} \left[\mathcal{L}_{\mathcal{A}1}^{(\alpha,\beta_1)}(\lambda) \dots \mathcal{L}_{\mathcal{A}L-1}^{(\alpha,\beta_{L-1})}(\lambda) \mathcal{L}_{\mathcal{A}L}^{(\alpha,\beta_L)}(\lambda) \right]. \tag{11}$$

Here we can see that, due to unitarity (7), the logarithmic derivative results in the same Hamiltonian $\overline{\mathcal{H}} = \mathcal{H}$ and $\overline{T}(0)$ corresponds to the left multiple-step shift operator, such that $T(0)\overline{T}(0) = \mathcal{N}\,\mathrm{Id}$ where $\mathcal{N} = \prod_{i=1}^{L} \zeta_{\alpha,\beta_i}(0)$.

In analogy to (6), we can write the transfer matrix $\overline{T}(\lambda)$ as

$$\overline{T}(\lambda) = \overline{T}(0) e^{\lambda\mathcal{H} + O(\lambda^2)}. \tag{12}$$

Using (6) and (12) we can rewrite the partition function Z in terms of the transfer matrices $T(\lambda)$ and $\overline{T}(\lambda)$ by considering the Trotter limit,

$$\begin{aligned} Z &= \lim_{N\to\infty} \mathrm{Tr}\left[(e^{-\frac{2\beta}{N}\mathcal{H}})^{N/2} \right], && (13)\\ &= \lim_{N\to\infty} \mathrm{Tr}\left[\left(T(-\tau)\overline{T}(-\tau) \right)^{N/2} \right] \frac{1}{\mathcal{N}^{N/2}}, \qquad \tau := \frac{\beta}{N}. && (14) \end{aligned}$$

The partition function (14) can be related to a staggered vertex model with alternating rows T and $\overline{T}$. In this case we need to know all the eigenvalues of these two transfer matrices to obtain the partition function in a

closed form. This is due to the fact that the eigenvalues of both transfer matrices depend on the length of the quantum chain L and in particular on the Trotter number N, such that for $N \to \infty$ all gaps close. However, we can circumvent this problem by rewriting (14) in terms of the column-to-column transfer matrix describing transfer in chain direction and hence is called the quantum transfer matrix

$$\begin{aligned}\frac{T_i^{QTM}(x)}{(\varsigma_{\alpha,\beta_i}(-(\mathrm{i}x+\tau)))^{N/2}} &= \mathrm{Tr}_{V_i}\,[\mathcal{L}_{V_iN}^{(\beta_i,\alpha)}(\mathrm{i}x+\tau-\rho)\mathcal{L}_{V_iN-1}^{(\beta_i,\alpha)}(\mathrm{i}x-\tau) \\ &\quad \ldots \mathcal{L}_{V_i2}^{(\beta_i,\alpha)}(\mathrm{i}x+\tau-\rho)\mathcal{L}_{V_i1}^{(\beta_i,\alpha)}(\mathrm{i}x-\tau)]. \end{aligned} \tag{15}$$

Each of these objects has a well defined largest eigenvalue separated by a gap from the rest of the spectrum, even in the limit $N \to \infty$. Therefore, only the largest eigenvalue is required for the computation of the partition function. Here x is the spectral parameter associated with the vertical line ensuring the existence of a commuting family of matrices, $\left[T_i^{QTM}(x), T_i^{QTM}(x')\right] = 0$. However, of direct physical relevance is $x = 0$ for obtaining the partition function,

$$Z = \lim_{N\to\infty} \mathrm{Tr}\left[\prod_{i=1}^{L} T_i^{QTM}(0)\right]\frac{1}{\mathcal{N}^{N/2}}. \tag{16}$$

Next, we address the identification of the largest eigenvalue of the product of the quantum transfer matrices $T_i^{QTM}(x)$. In general, the determination of the largest eigenvalue of the product of matrices $\prod_{i=1}^{L} T_i^{QTM}(x)$ would require the knowledge of all the eigenvalues of all transfer matrices $T_i^{QTM}(x)$, which could turn out to be a more involved problem than the staggered model mentioned above.

Nevertheless, this problem can be overcome under certain conditions. For instance, for the case of mixed spin chains all of the transfer matrices

commute according to the Yang-Baxter equation and the largest eigenvalues of the individual transfer matrices correspond to the same eigenvector. This implies that the largest eigenvalue of the product of L different transfer matrices is nothing than the product of the largest eigenvalues of the quantum transfer matrices. In this work, we will restrict to this specific case.

Here we are interested in the free energy and its derivatives, so we have to consider the logarithm of the partition function in the infinite length limit. As the eigenvalues $\Lambda_i^{QTM}(x)$ depend only on the Trotter number, we can first take the infinite length limit and later the infinite Trotter number limit, which reads

$$f = -\frac{1}{\beta} \lim_{L,N\to\infty} \frac{1}{L} \ln{[Z]}, \tag{17}$$

$$= -\frac{1}{\beta} \lim_{N,L\to\infty} \frac{1}{L} \sum_{i=1}^{L} \ln\left[\Lambda_{i,max}^{QTM}(0)\right] + \frac{1}{\beta} \lim_{N,L\to\infty} \frac{1}{L} \ln\left[\mathcal{N}^{N/2}\right]. \tag{18}$$

Before closing this section, we would like to mention that the properties (7-9) are also satisfied by many isomorphic self-crossed models [21]. For the $SU(N)$ case with $N > 2$, the property (9) reduces to the standard "rotation" of the vertex configuration of the Boltzmann weights.

3 Alternating spin chains

In the previous section, we used unitarity, time reversal and crossing properties to construct the quantum transfer matrix considering general representations of $\mathcal{L}_{\mathcal{A}i}^{(\alpha,\beta_i)}(\lambda)$. From now on, we consider (for an even number of lattice sites L) the alternation of two different representations of the group $SU(2)$ with spin S_1 at odd sites and spin S_2 at even sites, i.e. $\beta_{2i-1} = S_1$

and $\beta_{2i} = S_2$. In order to have a Hamiltonian with local interactions we fix α to be identical to the spin S_1 representation (equivalently we could have chosen S_2).

The monodromy matrix (1) becomes

$$\mathcal{T}_{\mathcal{A}}^{(S_1,S_2)}(\lambda) = \mathcal{L}_{\mathcal{A}L}^{(S_1,S_2)}(\lambda)\mathcal{L}_{\mathcal{A}L-1}^{(S_1,S_1)}(\lambda)\dots\mathcal{L}_{\mathcal{A}2}^{(S_1,S_2)}(\lambda)\mathcal{L}_{\mathcal{A}1}^{(S_1,S_1)}(\lambda), \tag{19}$$

with the auxiliary space $\mathcal{A} \equiv \mathbb{C}^{2S_1+1}$, and $\mathcal{L}_{\mathcal{A}i}^{(S_1,S_2)}(\lambda)$ resp. $\mathcal{L}_{\mathcal{A}i}^{(S_1,S_1)}(\lambda)$ are the $\mathcal{L}$-operators with spin S_1 representation in the auxiliary space and S_2 resp. S_1 in the quantum space.

The above $SU(2)$ invariant $\mathcal{L}$-operators can be obtained through the fusion process [22]. Its explicit form conveniently normalized is given by

$$\mathcal{L}_{12}^{(S_1,S_2)}(\lambda) = \sum_{l=|S_1-S_2|}^{S_1+S_2} f_l(\lambda)\check{P}_l, \tag{20}$$

where[1] $f_l(\lambda) = \prod_{j=l+1}^{S_1+S_2}\left(\frac{\lambda-j}{\lambda+j}\right)\prod_{j=1}^{*2S_1}(\lambda+S_2-S_1+j)$ and $\check{P}_l$ is the projector onto the $SU(2)_l$ in the Clebsch-Gordon decomposition $SU(2)_{S_1}\otimes SU(2)_{S_2}$. This operator is represented by

$$\check{P}_l = \prod_{\substack{k=|S_1-S_2|\\k\neq l}}^{S_1+S_2} \frac{\vec{S}_1\otimes\vec{S}_2 - x_k}{x_l - x_k}, \tag{21}$$

with $x_l = \frac{1}{2}\left[l(l+1) - S_1(S_1+1) - S_2(S_2+1)\right]$ and the $SU(2)$ generators $\vec{S}_a = (\hat{S}_a^x, \hat{S}_a^y, \hat{S}_a^z)$ for $a = 1, 2$.

The operator (20) is a solution of (3) with the following R-matrix

$$R_{12}^{(S_1)}(\lambda) = P_{12}\mathcal{L}_{12}^{(S_1,S_1)}(\lambda). \tag{22}$$

[1]The symbol $*$ shall remind that the possibility $j = S_1 - S_2$ is excluded throughout this work.

It satisfies the properties (7-9) with scalar functions given by $\zeta_{S_1,S_2}(\lambda) = \prod_{j=1}^{2S_1}((S_2 - S_1 + j)^2 - \lambda^2)$ and $\varsigma_{S_1,S_2}(\lambda) = (-1)^{2S_1}$ and crossing parameter $\rho = 1$. The matrix M is an anti-diagonal matrix whose non-zero elements are $M_{i,j} = -(-1)^i \delta_{i,2S_1+2-j}$.

The Hamiltonian associated to the transfer matrix $T(\lambda) = \mathrm{Tr}_{\mathcal{A}}\left[\mathcal{T}_{\mathcal{A}}^{(S_1,S_2)}(\lambda)\right]$ has terms with two and three site interactions. Its generic expression is given by

$$\begin{aligned} \mathcal{H}^{(S_1,S_2)} &= \sum_{\text{even } i} \left[\mathcal{L}_{i-1,i}^{(S_1,S_2)}(0)\right]^{-1} \frac{\partial}{\partial\lambda}\mathcal{L}_{i-1,i}^{(S_1,S_2)}(\lambda)\Big|_{\lambda=0} \\ &+ \sum_{\text{odd } i} \left[\mathcal{L}_{i-2,i-1}^{(S_1,S_2)}(0)\right]^{-1} \left[\mathcal{L}_{i-2,i}^{(S_1,S_1)}(0)\right]^{-1} \frac{\partial}{\partial\lambda}\mathcal{L}_{i-2,i}^{(S_1,S_1)}(\lambda)\Big|_{\lambda=0} \mathcal{L}_{i-2,i-1}^{(S_1,S_2)}(0), \end{aligned} \tag{23}$$

where periodic boundary conditions are assumed. For illustration, the Hamiltonian for case $S_1 = 1/2$, $S_2 = S$ is given explicitly by [15]

$$\begin{aligned} \mathcal{H}^{(\frac{1}{2},S)} &= \frac{1}{2}\left(\frac{1}{S+\frac{1}{2}}\right)^2 \Big[\sum_{\text{even } i} \left(\vec{\sigma}_{i-1}\cdot\vec{S}_i + \vec{S}_i\cdot\vec{\sigma}_{i+1} + \left\{\vec{\sigma}_{i-1}\cdot\vec{S}_i, \vec{S}_i\cdot\vec{\sigma}_{i+1}\right\}\right) \\ &+ \left(\frac{1}{4} - S(S+1)\right) \sum_{\text{even } i} \vec{\sigma}_{i-1}\cdot\vec{\sigma}_{i+1}\Big] + \frac{L}{4}\left(1 + \frac{1}{(S+\frac{1}{2})^2}\right). \end{aligned} \tag{24}$$

One of the consequences of the alternation of two different spins is that we have two quantum transfer matrices to work with. We denote them by $T^{(S_1)}(x)$ and $T^{(S_2)}(x)$, such as

$$\begin{aligned} T^{(S_a)}(x) &:= T_a^{QTM}(x) = \mathrm{Tr}_{V_a}\,[\mathcal{L}_{V_aN}^{(S_a,S_1)}(\mathrm{i}x+\tau-\rho)\mathcal{L}_{V_aN-1}^{(S_a,S_1)}(\mathrm{i}x-\tau) \\ &\quad \ldots \mathcal{L}_{V_a2}^{(S_a,S_1)}(\mathrm{i}x+\tau-\rho)\mathcal{L}_{V_a1}^{(S_a,S_1)}(\mathrm{i}x-\tau)], \end{aligned} \tag{25}$$

where the vertical spaces are $V_a \equiv \mathbb{C}^{2S_a+1}$ and $a = 1, 2$.

The transfer matrices (25) for $a = 1, 2$ commute due to the Yang-Baxter relation [23]. Therefore, they can be diagonalized simultaneously. It can also

be deduced from [23] that their largest eigenvalues correspond to the same eigenstate. Hence the largest eigenvalue of the product $T^{(S_1)}(x)T^{(S_2)}(x)$ is the product of the largest eigenvalues of $T^{(S_1)}(x)$ and $T^{(S_2)}(x)$.

For the analysis of the spectra we use the fusion hierarchy for the quantum transfer matrix $T^{(j)}(x)$, in analogy to the fusion of $\mathcal{L}$-operators. The algebraic relations read (see e.g. [10])

$$T^{(j)}(x)T^{(\frac{1}{2})}(x+\mathrm{i}(j+\frac{1}{2})) = a_j(x)T^{(j+\frac{1}{2})}(x+\frac{\mathrm{i}}{2}) + a_{j+1}(x)T^{(j-\frac{1}{2})}(x-\frac{\mathrm{i}}{2}),$$
$$T^{(0)}(x) = a_0(x)\mathrm{Id}, \quad j=\frac{1}{2},1,\frac{3}{2},\dots \tag{26}$$

where $a_j(x) = \prod_{l=1}^{2S_1} \phi_+(x+\mathrm{i}(j-S_1+l-1))\phi_-(x+\mathrm{i}(j-S_1+l))$ and $\phi_\pm(x) = (x \pm \mathrm{i}\tau)^{N/2}$.

From the fusion hierarchy with bilinear and linear expressions in T (26), one can obtain another set of functional relations [24], usually called T-system, with exclusively bilinear expressions

$$T^{(j)}(x+\frac{\mathrm{i}}{2})T^{(j)}(x-\frac{\mathrm{i}}{2}) = T^{(j-\frac{1}{2})}(x)T^{(j+\frac{1}{2})}(x) + f_j(x)\ \mathrm{Id}, \tag{27}$$

where $f_j(x) = \prod_{l=1}^{2S_1} \phi_+(x-\mathrm{i}(j-S_1+l+\frac{1}{2}))\phi_-(x-\mathrm{i}(j-S_1+l-\frac{1}{2}))\phi_+(x+\mathrm{i}(j-S_1+l-\frac{1}{2}))\phi_-(x+\mathrm{i}(j-S_1+l+\frac{1}{2}))$ for any j integer or semi-integer.

Equally important is a set of functional relations referred to as the Y-system, which is a consequence of (27). It is written as

$$y^{(j)}(x+\frac{\mathrm{i}}{2})y^{(j)}(x-\frac{\mathrm{i}}{2}) = Y^{(j-\frac{1}{2})}(x)Y^{(j+\frac{1}{2})}(x), \tag{28}$$

where $y^{(j)}(x) = \frac{T^{(j-\frac{1}{2})}(x)T^{(j+\frac{1}{2})}(x)}{f_j(x)}$ and $Y^{(j)}(x) = 1 + y^{(j)}(x)$.

Lastly, we introduce a Zeeman term $\widetilde{\mathcal{H}} = \mathcal{H} - h\hat{S}^z$. This term represents the coupling of the magnetic field h to the spin $\hat{S}^z = \sum_{\substack{i=1 \\ \text{odd } i}}^{L} \hat{S}^z_{1,i} + \sum_{\substack{i=1 \\ \text{even } i}}^{L} \hat{S}^z_{2,i}$.

It can be introduced inside the trace of the partition function such as,

$$Z = \lim_{N\to\infty} \mathrm{Tr}\left[\left(T(-\tau)\overline{T}(-\tau)\right)^{N/2} e^{\beta h \hat{S}^z}\right]\frac{1}{\mathcal{N}^{N/2}}. \tag{29}$$

Alternatively, it can be considered as a diagonal boundary term on the vertical lines along a horizontal seam. This redefines only trivially the quantum transfer matrix

$$\begin{aligned} T^{(S_a)}(x) &= \mathrm{Tr}_{V_a}\,[\mathcal{G}_a\mathcal{L}^{(S_a,S_1)}_{V_aN}(\mathrm{i}x+\tau-\rho)\mathcal{L}^{(S_a,S_1)}_{V_aN-1}(\mathrm{i}x-\tau) \\ &\quad \ldots \mathcal{L}^{(S_a,S_1)}_{V_a2}(\mathrm{i}x+\tau-\rho)\mathcal{L}^{(S_a,S_1)}_{V_a1}(\mathrm{i}x-\tau)], \end{aligned} \tag{30}$$

where $\mathcal{G}_a$ is a diagonal matrix whose non-zero elements are $(\mathcal{G}_a)_{i,i} = e^{\beta h(S_a+1-i)}$.

The eigenvalues $\Lambda^{(j)}(x)$ associated to $T^{(j)}(x)$ also satisfy the functional relations (26-28). This is due to the commutativity property among different $T^{(j)}(x)$. This way, we obtain the eigenvalues at any fusion level in terms of the first level eigenvalue through the iteration of the relations (26) and (27). Alternatively, we can proceed along the same lines as [25] applying the algebraic Bethe ansatz to the case of twisted boundary conditions.

In both cases we end up with the eigenvalues of the quantum transfer matrix (30),

$$\Lambda^{(j)}(x) = \sum_{m=1}^{2j+1} \lambda_m^{(j,S_1)}(x), \tag{31}$$

$$\lambda_m^{(j)}(x) = e^{\beta h(j+1-m)} t^{(j)}_{+,m}(x) t^{(j)}_{-,m}(x+\mathrm{i}) \frac{Q(x-\mathrm{i}(\frac{1}{2}+j))Q(x+\mathrm{i}(\frac{1}{2}+j))}{Q(x-\mathrm{i}(\frac{3}{2}+j-m))Q(x-\mathrm{i}(\frac{1}{2}+j-m))}, \tag{32}$$

where $t^{(j)}_{\pm,m}(x) = \prod_{l=j-m+2}^{j} \frac{\phi_\pm(x-\mathrm{i}(l-S_1))}{\phi_\pm(x-\mathrm{i}(l+S_1))} \prod_{l=1}^{2S_1}{}^{*}\, \phi_\pm(x-\mathrm{i}(j-S_1+l))$ and $Q(x) =$

$\prod_{l=1}^{n}(x-x_l)$. The corresponding Bethe ansatz equations can be written as

$$e^{\beta h}\frac{\phi_+(x_l-\mathrm{i}(S_1+\frac{1}{2}))\phi_-(x_l-\mathrm{i}(S_1-\frac{1}{2}))}{\phi_-(x_l+\mathrm{i}(S_1+\frac{1}{2}))\phi_+(x_l+\mathrm{i}(S_1-\frac{1}{2}))}=\prod_{\substack{j=1\\ j\neq l}}^{n}\frac{x_l-x_j-\mathrm{i}}{x_l-x_j+\mathrm{i}}. \tag{33}$$

According to the previous section, we only need to know the largest eigenvalue in the limit $N\to\infty$ to describe the thermodynamics of the one dimensional quantum model. Then for instance by numerical analysis of the Bethe ansatz equation (33) for small N we see that the largest eigenvalue lies in the sector $n=S_1N$. However, the limit $N\to\infty$ cannot be considered numerically. So, we need to encode the Bethe ansatz roots in such a way that the free energy can be evaluated independently of the exact knowledge of the individual roots.

One possible way is to define a set of suitable auxiliary functions depending on the Bethe ansatz roots. Then by exploiting the above and further functional relations we eliminate the explicit dependence on the roots. Therefore the Bethe ansatz roots for finite N (including the limit $N\to\infty$) become encoded in a finite set of auxiliary functions satisfying certain nonlinear integral equations.

Such an analysis was already done for many cases, for instance for the spin-1/2 Heisenberg chain [7, 8, 9] and its higher spin extensions [10]. In the latter case, the auxiliary functions were taken as a subset of the y-functions complemented by two "novel" functions which reduce the infinitely many functional relations (28) to finitely many. This is the starting point of the next section.

4 Non-linear integral equations

In this section, we introduce a suitable set of auxiliary functions and explore its analyticity properties to obtain a finite set of non-linear integral equations. These auxiliary functions turn out to describe the largest eigenvalue of (30) and consequently the free energy (18) at finite temperature. Specifically, we need to define $2s+1$ auxiliary functions, where $s = \max(S_1, S_2)$. We will proceed along the lines of [10] and take as the first $2s-1$ auxiliary functions the y-functions

$$y^{(j)}(x) = \frac{\Lambda^{(j-\frac{1}{2})}(x)\Lambda^{(j+\frac{1}{2})}(x)}{f_j(x)}, \quad j = \frac{1}{2}, \dots, s - \frac{1}{2}. \tag{34}$$

The two remaining functions are defined as

$$b(x) = \frac{\lambda_1^{(s)}(x+\frac{\mathrm{i}}{2}) + \dots + \lambda_{2s}^{(s)}(x+\frac{\mathrm{i}}{2})}{\lambda_{2s+1}^{(s)}(x+\frac{\mathrm{i}}{2})}, \tag{35}$$

$$\bar{b}(x) = \frac{\lambda_2^{(s)}(x-\frac{\mathrm{i}}{2}) + \dots + \lambda_{2s+1}^{(s)}(x-\frac{\mathrm{i}}{2})}{\lambda_1^{(s)}(x-\frac{\mathrm{i}}{2})}. \tag{36}$$

In addition to this, we introduce a shorthand notation for simply related functions $B(x) := 1 + b(x)$, $\bar{B}(x) := 1 + \bar{b}(x)$ and $Y^{(j)}(x) := 1 + y^{(j)}(x)$ for $j = \frac{1}{2}, \dots, s - \frac{1}{2}$.

In conformity with the previous definition, we note that $B(x) = \frac{\Lambda^{(s)}(x+\frac{\mathrm{i}}{2})}{\lambda_{2s+1}^{(s)}(x+\frac{\mathrm{i}}{2})}$ and $\bar{B}(x) = \frac{\Lambda^{(s)}(x-\frac{\mathrm{i}}{2})}{\lambda_1^{(s)}(x-\frac{\mathrm{i}}{2})}$ with product $B(x)\bar{B}(x) = Y^{(s)}(x)$. This implies for the first $(2s-1)$ functional relations (28)

$$y^{(j)}(x+\frac{\mathrm{i}}{2})y^{(j)}(x-\frac{\mathrm{i}}{2}) = Y^{(j-\frac{1}{2})}(x)Y^{(j+\frac{1}{2})}(x) \text{ for } j = \frac{1}{2}, 1, \dots, s-1, \tag{37}$$

$$y^{(s-\frac{1}{2})}(x+\frac{\mathrm{i}}{2})y^{(s-\frac{1}{2})}(x-\frac{\mathrm{i}}{2}) = Y^{(s-1)}(x)B(x)\bar{B}(x). \tag{38}$$

We can write $b(x), \bar{b}(x), B(x)$ and $\bar{B}(x)$ explicitly using (32) such that

$$b(x) = \frac{Q(x+\mathrm{i}(s+1))}{Q(x-\mathrm{i}s)} \frac{e^{\beta h(s+\frac{1}{2})}\Lambda^{(s-\frac{1}{2})}(x)}{\prod_{l=1}^{2S_1}\phi_+(x+\mathrm{i}(s-S_1+l-\frac{1}{2}))\phi_-(x+\mathrm{i}(s-S_1+l+\frac{1}{2}))}, \tag{39}$$

$$\bar{b}(x) = \frac{Q(x-\mathrm{i}(s+1))}{Q(x+\mathrm{i}s)} \frac{e^{-\beta h(s+\frac{1}{2})}\Lambda^{(s-\frac{1}{2})}(x)}{\prod_{l=1}^{2S_1}\phi_+(x-\mathrm{i}(s-S_1+l+\frac{1}{2}))\phi_-(x-\mathrm{i}(s-S_1+l-\frac{1}{2}))}, \tag{40}$$

$$B(x) = \frac{Q(x+\mathrm{i}s)}{Q(x-\mathrm{i}s)} \frac{e^{\beta hs}\Lambda^{(s)}(x+\frac{\mathrm{i}}{2})}{\prod_{l=1}^{2S_1}\phi_+(x+\mathrm{i}(s-S_1+l-\frac{1}{2}))\phi_-(x+\mathrm{i}(s-S_1+l+\frac{1}{2}))}, \tag{41}$$

$$\bar{B}(x) = \frac{Q(x-\mathrm{i}s)}{Q(x+\mathrm{i}s)} \frac{e^{-\beta hs}\Lambda^{(s)}(x-\frac{\mathrm{i}}{2})}{\prod_{l=1}^{2S_1}\phi_+(x-\mathrm{i}(s-S_1+l+\frac{1}{2}))\phi_-(x-\mathrm{i}(s-S_1+l-\frac{1}{2}))}. \tag{42}$$

In this way, it is evident that $b(x)$, $\bar{b}(x)$ are related to $\Lambda^{(s-\frac{1}{2})}(x)$.

Moreover, $\Lambda^{(s-\frac{1}{2})}(x)$ is related to $Y^{(s-\frac{1}{2})}(x)$ through the definition of y-function. This relation can be written as

$$\Lambda^{(s-\frac{1}{2})}(x+\frac{\mathrm{i}}{2})\Lambda^{(s-\frac{1}{2})}(x-\frac{\mathrm{i}}{2}) = f_{s-\frac{1}{2}}(x)Y^{(s-\frac{1}{2})}(x). \tag{43}$$

At this point, we have a common set of functions which still depend on the Bethe ansatz roots and whose limit $N \to \infty$ is still to be performed. However, this dependence as well as the limit can be worked out easily in Fourier space.

In order to calculate the Fourier transform, we exploit the analyticity properties of the eigenvalue of the quantum transfer matrix and the auxiliary functions. Furthermore, these functions should be non-zero and have constant asymptotics in a strip around the real axis. This allows us to apply

the Fourier transform to the logarithmic derivative of the auxiliary functions,

$$\hat{f}(k) = \int_{-\infty}^{\infty} \frac{d}{dx} \left[\ln f(x)\right] e^{-\mathrm{i}kx} \frac{dx}{2\pi}. \tag{44}$$

In the cases $k < 0$ and $k > 0$, we have chosen a closed contour above and below the real axis, respectively. For this reason, it is of fundamental importance to analyze the structure of the zeros of the auxiliary functions.

In particular, the zeros and poles of the auxiliary functions (34-36) originate from the zeros of $Q(x)$ and $\Lambda^{(j)}(x)$ for $j = \frac{1}{2}, \dots, s$ besides those of the $\phi_{\pm}(x)$ functions. Therefore, we have to analyze the qualitative distribution of the Bethe ansatz roots as well as the zeros of the eigenvalue functions $\Lambda^{(j)}(x)$.

It is well known that Bethe ansatz roots form $2S_1$-strings in the particle sector $n = S_1 N$. These roots have imaginary parts placed approximately at $(S_1 + \frac{1}{2} - l)$ for $l = 1, \dots, 2S_1$ [23]. Concerning the zeros of $\Lambda^{(j)}(x)$ for $j = \frac{1}{2}, \dots, s$, we have verified numerically that their imaginary parts are placed at $\pm(j - S_1 + l)$ for $l = 1, \dots, 2S_1$ and $l \neq S_1 - j$.

By direct inspection of (34,37-43), we note that almost all auxiliary functions are free of zeros and poles in a strip containing $-1/2 \leq \Im(x) \leq 1/2$. The exceptions are $y^{(S_1)}(x)$ for $S_1 < S_2$ and $b(x), \bar{b}(x)$ for $S_1 \geq S_2$, which should be treated separately.

This way, the position of the zeros and poles of the auxiliary functions depend on the relative magnitude of S_1 and S_2. So, we have to split our analysis in three parts: $S_1 < S_2$, $S_1 = S_2$ and $S_1 > S_2$.

4.1 $S_1 < S_2$

In this case, we have $s = S_2$ in the previous definition. In order to deal with the problem involving the function $y^{(S_1)}(x)$, we define a related function for which the problematic zeros and poles at $x = \pm\mathrm{i}/2$ are cancelled,

$$\tilde{y}^{(S_1)}(x) = \frac{\phi_+(x+\frac{\mathrm{i}}{2})\phi_-(x-\frac{\mathrm{i}}{2})}{\phi_-(x+\frac{\mathrm{i}}{2})\phi_+(x-\frac{\mathrm{i}}{2})} y^{(S_1)}(x). \quad (45)$$

Consequently, the $2S_1$-th equation in (37) becomes

$$\tilde{y}^{(S_1)}(x+\frac{\mathrm{i}}{2})\tilde{y}^{(S_1)}(x-\frac{\mathrm{i}}{2}) = \frac{\phi_-(x-\mathrm{i})\phi_+(x+\mathrm{i})}{\phi_+(x-\mathrm{i})\phi_-(x+\mathrm{i})} Y^{(S_1-\frac{1}{2})}(x)Y^{(S_1+\frac{1}{2})}(x), \quad (46)$$

and the functions $\tilde{y}^{(S_1)}(x \pm \frac{\mathrm{i}}{2})$ can be transformed as usual according to (44). On the other hand, we can apply the Fourier transform to the equation (45), once it does not have zeros and poles on the real axis. Thus we are able to establish a relation between $y^{(S_1)}$ and $\tilde{y}^{(S_1)}$ in Fourier space,

$$\hat{\tilde{y}}^{(S_1)}(k) = \mathrm{i}N \sinh[k\beta/N] e^{-|k|/2} + \hat{y}^{(S_1)}(k). \quad (47)$$

Now, applying (44) to the functional relations (37-43) and (46) we obtain after a long but straightforward calculation a set of algebraic relations in Fourier space. These relation are given in terms of the transformed auxiliary functions $\hat{y}^{(j)}(k)$, $\hat{b}(k)$, $\hat{\bar{b}}(k)$, $\hat{Y}^{(j)}(k)$, $\hat{B}(k)$, $\hat{\bar{B}}(k)$ and the unknowns $\hat{\Lambda}^{(S_2-\frac{1}{2})}(k)$, $\hat{\Lambda}^{(S_2)}(k)$ and $\hat{Q}(k)$. We can eliminate the unknowns after some

algebraic manipulation. Finally, using (47) we obtain

$$\begin{pmatrix} \hat{y}^{(\frac{1}{2})}(k) \\ \vdots \\ \hat{y}^{(S_1)}(k) \\ \vdots \\ \hat{y}^{(S_2-\frac{1}{2})}(k) \\ \hat{b}(k) \\ \hat{\bar{b}}(k) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \hat{d}(k) \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix} + \hat{\mathcal{K}}(k) \begin{pmatrix} \hat{Y}^{(\frac{1}{2})}(k) \\ \vdots \\ \hat{Y}^{(S_1)}(k) \\ \vdots \\ \hat{Y}^{(S_2-\frac{1}{2})}(k) \\ \hat{B}(k) \\ \hat{\bar{B}}(k) \end{pmatrix}, \tag{48}$$

where the kernel $\hat{\mathcal{K}}(k)$ is a $(2S_2+1)\times(2S_2+1)$ matrix given by

$$\hat{\mathcal{K}}(k) = \begin{pmatrix} 0 & \hat{K}(k) & 0 & \cdots & & 0 & 0 & 0 & 0 \\ \hat{K}(k) & 0 & \hat{K}(k) & & & \vdots & \vdots & \vdots & \vdots \\ 0 & \hat{K}(k) & 0 & & & & 0 & 0 & 0 \\ \vdots & & & & & 0 & \hat{K}(k) & 0 & 0 \\ 0 & 0 & \cdots & & 0 & \hat{K}(k) & 0 & \hat{K}(k) & \hat{K}(k) \\ 0 & 0 & \cdots & & 0 & 0 & \hat{K}(k) & \hat{F}(k) & -e^{-k}\hat{F}(k) \\ 0 & 0 & \cdots & & 0 & 0 & \hat{K}(k) & -e^{k}\hat{F}(k) & \hat{F}(k) \end{pmatrix}, \tag{49}$$

with $\hat{K}(k) = \frac{1}{2\cosh[k/2]}$, $\hat{F}(k) = \frac{e^{-|k|/2}}{2\cosh[k/2]}$ and $\hat{d}(k) = -\mathrm{i}N\frac{\sinh[k\beta/N]}{2\cosh[k/2]}$.

As the Trotter number N appears only in $\hat{d}(k)$, we can take the limit $N\to\infty$ straightforwardly,

$$\hat{d}(k) = -\frac{\mathrm{i}}{2\cosh[k/2]}\lim_{N\to\infty} N\sinh[k\beta/N] = -\frac{\mathrm{i}k\beta}{2\cosh[k/2]}. \tag{50}$$

The inverse Fourier transform has been applied to (48) followed by an

integration over x, resulting in

$$\begin{pmatrix} \ln y^{(\frac{1}{2})}(x) \\ \vdots \\ \ln y^{(S_1)}(x) \\ \vdots \\ \ln y^{(S_2-\frac{1}{2})}(x) \\ \ln b(x) \\ \ln \bar{b}(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ -\beta d(x) \\ \vdots \\ 0 \\ \beta\frac{h}{2} \\ -\beta\frac{h}{2} \end{pmatrix} + \mathcal{K} * \begin{pmatrix} \ln Y^{(\frac{1}{2})}(x) \\ \vdots \\ \ln Y^{(S_1)}(x) \\ \vdots \\ \ln Y^{(S_2-\frac{1}{2})}(x) \\ \ln B(x) \\ \ln \bar{B}(x) \end{pmatrix}, \qquad (51)$$

where $d(x) = \frac{\pi}{\cosh[\pi x]}$ and the symbol $*$ denotes the convolution $f * g(x) = \int_{-\infty}^{\infty} f(x-y)g(y)dy$. The integration constants $\pm\beta h/2$ were determined in the asymptotic limit $|x| \to \infty$.

The kernel matrix is given explicitly by

$$\mathcal{K}(x) = \begin{pmatrix} 0 & K(x) & 0 & \cdots & & 0 & 0 & 0 & 0 \\ K(x) & 0 & K(x) & & & \vdots & \vdots & \vdots & \vdots \\ 0 & K(x) & 0 & & & & 0 & 0 & 0 \\ \vdots & & & & & 0 & K(x) & 0 & 0 \\ 0 & 0 & \cdots & & 0 & K(x) & 0 & K(x) & K(x) \\ 0 & 0 & \cdots & & 0 & 0 & K(x) & F(x) & -F(x+\mathrm{i}) \\ 0 & 0 & \cdots & & 0 & 0 & K(x) & -F(x-\mathrm{i}) & F(x) \end{pmatrix}, \qquad (52)$$

where $K(x) = \frac{\pi}{\cosh[\pi x]}$ and $F(x) = \int_{-\infty}^{\infty} \frac{e^{-|k|/2+\mathrm{i}kx}}{2\cosh[k/2]} dk$.

Now, we have to derive an expression for the eigenvalue $\Lambda^{(S_2)}(x)$ in terms of the auxiliary functions. It is convenient to define a new function

$$\underline{\Lambda}^{(S_2)}(x) = \frac{\Lambda^{(S_2)}(x)}{\prod_{l=1}^{2S_1} \phi_+(x - \mathrm{i}(S_2 - S_1 + l))\phi_-(x + \mathrm{i}(S_2 - S_1 + l))}, \qquad (53)$$

which has constant asymptotics. For $x=0$ and finite N, we have $\ln \Lambda^{(S_2)}(0) = \ln \underline{\Lambda}^{(S_2)}(0) + \sum_{l=1}^{2S_1} \ln \left[1 - \frac{\beta}{S_2-S_1+l}\frac{1}{N}\right]^N + \frac{2}{L}\ln\left[\mathcal{N}^{N/2}\right]$, where we have used the fact that $\mathcal{N} = \prod_{l=1}^{2S_1}(S_2-S_1+l)^L$.

Using the Fourier transformed version of (41-42,53), we obtain

$$\hat{\underline{\Lambda}}^{(S_2)}(k) = \mathrm{i}k\beta \frac{e^{-|k|(S_2-S_1-\frac{1}{2})}}{2\cosh[k/2]} \sum_{l=1}^{2S_1} e^{-|k|l} + \hat{K}(k)\left[\hat{B}(k) + \hat{\bar{B}}(k)\right]. \tag{54}$$

Proceeding as before, we apply the inverse Fourier transform followed by an integration over x and the determination of the integration constant. In this way, we obtain

$$\ln \underline{\Lambda}^{(S_2)}(x) = \beta\epsilon^{(S_2,S_1)}(x) + \left(K * \ln B\bar{B}\right)(x), \tag{55}$$

where $\epsilon^{(S_2,S_1)}(x)$ is given by

$$\epsilon^{(S_2,S_1)}(x) = \sum_{l=1}^{2S_1} \int_{-\infty}^{\infty} \frac{e^{-|k|(S_2-S_1+l-\frac{1}{2})}}{2\cosh[k/2]} e^{\mathrm{i}kx} dk. \tag{56}$$

At the point $x=0$, we can rewrite this integral in terms of the Euler psi function,

$$\epsilon^{(S_2,S_1)}(0) = \psi\left(\frac{S_2+S_1+1}{2}\right) - \psi\left(\frac{S_2-S_1+1}{2}\right). \tag{57}$$

The contribution of the quantum transfer matrix $T^{(S_2)}(0)$ (30) to the free energy is given by (18)

$$\begin{aligned} f^{(S_2,S_1)} &= -\frac{1}{2\beta}\lim_{N\to\infty} \ln\Lambda^{(S_2)}(0) + \frac{1}{\beta}\lim_{N,L\to\infty}\frac{1}{L}\ln\left[\mathcal{N}^{N/2}\right], & (58)\\ &= -\frac{1}{2\beta}\lim_{N\to\infty}\ln\underline{\Lambda}^{(S_2)}(0) + \frac{1}{2}\sum_{l=1}^{2S_1}\frac{1}{S_2-S_1+l}. & (59)\end{aligned}$$

Therefore, we can write $f^{(S_2,S_1)}$ explicitly as

$$\begin{aligned} f^{(S_2,S_1)} &= \frac{1}{2}\left[\sum_{l=1}^{2S_1}\frac{1}{S_2-S_1+l}-\psi\left(\frac{S_2+S_1+1}{2}\right)+\psi\left(\frac{S_2-S_1+1}{2}\right)\right] \\ & -\frac{1}{2\beta}\left(K*\ln B\bar{B}\right)(0). \end{aligned} \tag{60}$$

4.2 $S_1 = S_2$

In this case, we note that $b(x)$ and $\bar{b}(x)$ have zeros at $x = \pm\mathrm{i}/2$ which are presenting some subtleties. These zeros originate from the factor $\Lambda^{(S_1-\frac{1}{2})}$ and in principle do not present any problems for the computation of the Fourier transform of the logarithmic derivative of (39-40). The problem arises in the Fourier transform of (43), which is required to eliminate the unknown function $\Lambda^{(S_1-\frac{1}{2})}$.

Hence, we define a new function $\widetilde{\Lambda}^{(S_1-\frac{1}{2})}(x) = \frac{\Lambda^{(S_1-\frac{1}{2})}(x)}{\phi_+(x-\mathrm{i}/2)\phi_-(x+\mathrm{i}/2)}$, which does not have any zeros at $x = \pm\mathrm{i}/2$. We apply (44) to the functional relations (37-43) with $\widetilde{\Lambda}$ instead of Λ. Then we eliminate the unknowns $\hat{\Lambda}^{(S_1-\frac{1}{2})}(k)$ and $\hat{Q}(k)$ and finally we obtain

$$\begin{pmatrix} \hat{y}^{(\frac{1}{2})}(k) \\ \vdots \\ \hat{y}^{(S_1-\frac{1}{2})}(k) \\ \hat{b}(k) \\ \hat{\bar{b}}(k) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hat{d}(k) \\ \hat{d}(k) \end{pmatrix} + \hat{\mathcal{K}}(k) \begin{pmatrix} \hat{Y}^{(\frac{1}{2})}(k) \\ \vdots \\ \hat{Y}^{(S_1-\frac{1}{2})}(k) \\ \hat{B}(k) \\ \hat{\bar{B}}(k) \end{pmatrix}, \tag{61}$$

where the kernel $\hat{\mathcal{K}}(k)$ with the same structure as (49), is a $(2S_1+1)\times(2S_1+1)$ matrix.

Applying the inverse Fourier transform to (61) followed by an integration

over x, results in

$$\begin{pmatrix} \ln y^{(\frac{1}{2})}(x) \\ \vdots \\ \ln y^{(S_1-\frac{1}{2})}(x) \\ \ln b(x) \\ \ln \bar{b}(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -\beta d(x) + \beta\frac{h}{2} \\ -\beta d(x) - \beta\frac{h}{2} \end{pmatrix} + \mathcal{K} * \begin{pmatrix} \ln Y^{(\frac{1}{2})}(x) \\ \vdots \\ \ln Y^{(S_1-\frac{1}{2})}(x) \\ \ln B(x) \\ \ln \bar{B}(x) \end{pmatrix}, \quad (62)$$

where the $(2S_1+1) \times (2S_1+1)$ kernel matrix is given by (52).

Finally, the largest eigenvalue $\Lambda^{(S_1)}(0)$ of the quantum transfer matrix $T^{(S_1)}(0)$ (30) can be written in terms of the auxiliary functions in analogy to the previous case. We just have to set $S_2 = S_1$ in all expressions (53-60) and obtain,

$$\ln \underline{\Lambda}^{(S_1)}(0) = \beta \left[\psi\left(\frac{2S_1+1}{2}\right) - \psi\left(\frac{1}{2}\right)\right] + \left(K * \ln B\bar{B}\right)(0). \quad (63)$$

Its contribution to the free energy is given by

$$f^{(S_1,S_1)} = \frac{1}{2}\left[\sum_{l=1}^{2S_1} \frac{1}{l} - \psi\left(\frac{2S_1+1}{2}\right) + \psi\left(\frac{1}{2}\right)\right] - \frac{1}{2\beta}\left(K * \ln B\bar{B}\right)(0). \quad (64)$$

4.3 $S_1 > S_2$

For this case, the auxiliary functions as well as the set of non-linear integral equations are exactly the same as in the previous case $S_2 = S_1$. The only difference consists in the way how the largest eigenvalue $\Lambda^{(S_2)}(0)$ is expressed in terms of the auxiliary functions.

According to the definition of the Y-function, we have an equation similar to (43) which relates $\Lambda^{(S_2)}(x)$ and $Y^{(S_2)}(x)$. This relation can be written explicitly as

$$\Lambda^{(S_2)}(x + \frac{\mathrm{i}}{2})\Lambda^{(S_2)}(x - \frac{\mathrm{i}}{2}) = f_{S_2}(x) Y^{(S_2)}(x). \quad (65)$$

Applying (44) to (65,53), we obtain

$$\underline{\hat{\Lambda}}^{(S_2)}(k) = \frac{\mathrm{i}k\beta}{2\cosh[k/2]}\hat{\gamma}(k) + \hat{K}(k)\hat{Y}^{(S_2)}(k), \tag{66}$$

$$\hat{\gamma}(k) = \sum_{\substack{l=1 \\ l>(S_1-S_2)+a}}^{2S_1} e^{-|k|(S_2-S_1+l-\frac{1}{2})} - \sum_{\substack{l=1 \\ l<(S_1-S_2)-a}}^{2S_1} e^{-|k|(S_1-S_2-l+\frac{1}{2})} - e^{-|k|(\frac{1}{2}+a)}, \tag{67}$$

where $a = 0$ when $S_1 - S_2$ is an integer number and $a = 1/2$ when $S_1 - S_2$ is a half-integer number. Here, we recall that the possibility $l = S_1 - S_2$ was already excluded in the definition of the $\mathcal{L}$-operator (20).

After performing the inverse Fourier transform and integration over x, we obtain

$$\ln \underline{\Lambda}^{(S_2)}(x) = \beta\epsilon^{(S_1,S_2)}(x) + \left(K * \ln Y^{(S_2)}\right)(x), \tag{68}$$

with $\epsilon^{(S_1,S_2)}(x) = \int_{-\infty}^{\infty} \frac{\hat{\gamma}(k)e^{\mathrm{i}kx}dk}{2\cosh[k/2]}$. At the particular point $x = 0$, $\epsilon^{(S_1,S_2)}(x)$ is given by

$$\epsilon^{(S_1,S_2)}(0) = \psi\left(\frac{S_1+S_2+1}{2}\right) - \psi\left(\frac{S_1-S_2+1}{2}\right). \tag{69}$$

Lastly, the contribution to the free energy is written in terms of the auxiliary function

$$\begin{aligned} f^{(S_2,S_1)} &= \frac{1}{2}\left[\sum_{l=1}^{2S_1}{}^{*} \frac{1}{S_2-S_1+l} - \psi\left(\frac{S_1+S_2+1}{2}\right) + \psi\left(\frac{S_1-S_2+1}{2}\right)\right] \\ &\quad -\frac{1}{2\beta}\left(K * \ln Y^{(S_2)}\right)(0). \end{aligned} \tag{70}$$

It is interesting to compare $\epsilon^{(S_1,S_2)}(x)$ (69) with the previous cases (57,63). These expressions can be naturally written in a unified form as follows

$$\varepsilon^{(S_1,S_2)} = \epsilon^{(S_1,S_2)}(0) = \epsilon^{(S_2,S_1)}(0) = \psi\left(\frac{S_1+S_2+1}{2}\right) - \psi\left(\frac{|S_1-S_2|+1}{2}\right). \tag{71}$$

According to (18), the free energy of alternating spin chains is described by the sum of $\ln\Lambda^{(S_2)}(0)$ and $\ln\Lambda^{(S_1)}(0)$. As a result of that, the sum of $\varepsilon^{(S_1,S_2)}$ and $\varepsilon^{(S_1,S_1)}$ is the ground state energy of the quantum Hamiltonian $\mathcal{H}^{(S_1,S_2)}$,

$$\epsilon_0 = \psi\left(\frac{S_1+S_2+1}{2}\right) - \psi\left(\frac{|S_1-S_2|+1}{2}\right) + \psi\left(\frac{2S_1+1}{2}\right) - \psi\left(\frac{1}{2}\right), \quad (72)$$

which is in agreement with the results based on the $2S$-string hypothesis for the cases $S_1 = 1/2, S_2 = S$ [15] and $S_2 = S_1 = S$ [23].

The total free energy is the sum of two pieces $f = f^{(S_2,S_1)} + f^{(S_1,S_1)}$. As we have seen, the term $f^{(S_2,S_1)}$ at finite temperature can be written as

$$f^{(S_2,S_1)} = f_0^{(S_2,S_1)} - \frac{1}{2\beta}\begin{cases} \left(K * \ln B\bar{B}\right)(0), & \text{if } S_1 < S_2 \\ \left(K * \ln B\bar{B}\right)(0), & \text{if } S_1 = S_2 \\ \left(K * \ln Y^{(S_2,S_1)}\right)(0), & \text{if } S_1 > S_2, \end{cases} \quad (73)$$

where $f_0^{(S_2,S_1)} = \frac{1}{2}\left[\sum_{l=1}^{*2S_1} \frac{1}{S_2-S_1+l} - \varepsilon^{(S_2,S_1)}\right]$. Here we have to remind that all auxiliary functions, including $B(x)$ and $\bar{B}(x)$, are different for different cases $S_1 < S_2$ and $S_1 \geq S_2$.

We like to mention that results of an analysis similar to that above were published in [26] for the study of single Kondo impurities. In the present study of bulk properties of lattice models, the integral equations share some algebraic structures with those in [26], but have rather different analytic properties with respect to the driving terms.

5 Numerical results

In this section, we present the numerical results obtained for the specific heat and magnetic susceptibility for the cases $S_1 < S_2, S_1 = S_2$ and $S_1 > S_2$.

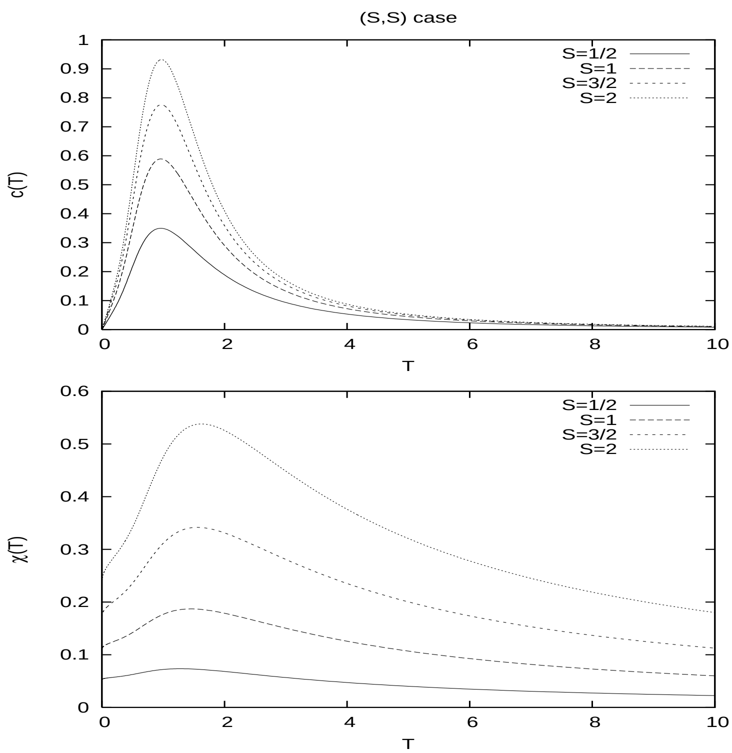

Figure 1: Specific heat $c(T)$ and $\chi(T)$ magnetic susceptibility versus temperature T for $S = 1/2, 1, 3/2, 2$.

We have solved numerically the non-linear integral equations by iteration. The convolutions have been calculated in Fourier space using the Fast Fourier Transform algorithm (FFT). Eventually, we have obtained the free energy as a function of temperature and magnetic field.

Instead of performing numerical differentiations to obtain the derivatives of the free energy with respect to temperature and magnetic field, we have used associated integral equations for the derivatives of the auxiliary functions. These integral equations arise from the differentiation of the set of

non-linear equations, e.g. with respect to the temperature T.

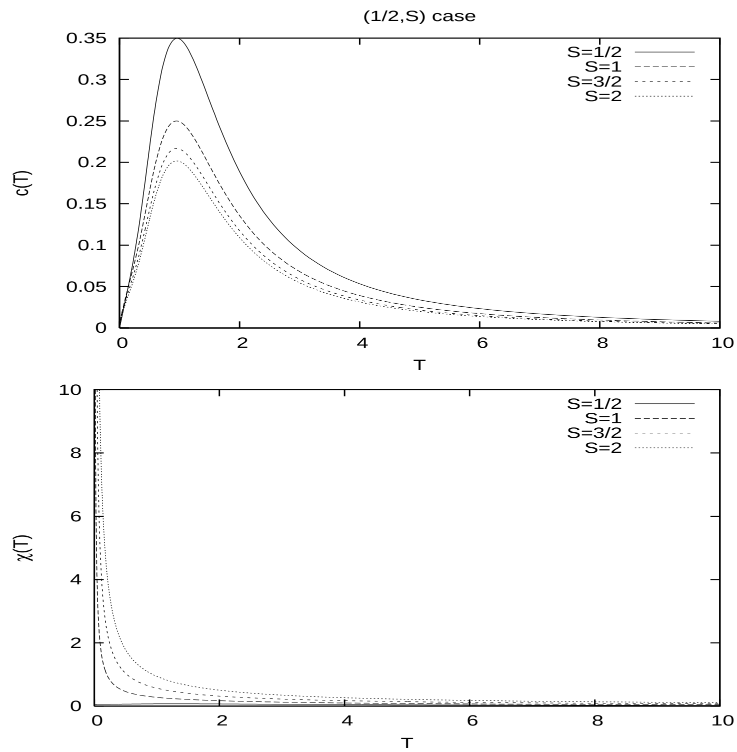

Figure 2: Specific heat $c(T)$ and $\chi(T)$ magnetic susceptibility versus temperature T for $S_1 = 1/2$ and $S_2 = S = 1/2, 1, 3/2, 2$.

Lastly, we have used the relation among the derivatives of the auxiliary functions reading

$$\frac{\partial}{\partial T} \ln B(x) = \frac{b(x)}{1+b(x)} \frac{\partial}{\partial T} \ln b(x), \tag{74}$$

$$\frac{\partial^2}{\partial T^2} \ln B(x) = \frac{b(x)}{1+b(x)} \left[\frac{1}{1+b(x)} \left(\frac{\partial}{\partial T} \ln b(x) \right)^2 + \frac{\partial^2}{\partial T^2} \ln b(x) \right]. \tag{75}$$

This way, we obtained for each increment in the order of differentiation a

new set of linear integral equations, where the lower order derivatives appear just as coefficients.

In Figures 1-3, we show the specific heat and the magnetic susceptibility as functions of temperature for the particular cases $S_1 = S_2 = S$, $S_1 = 1/2, S_2 = S$ and $S_1 = S, S_2 = 1/2$ for $S = 1/2, 1, 3/2, 2$, respectively.

The system shows antiferromagnetic behaviour for the first case $S_1 = S_2$. At low temperature $c(T)$ presents a linear temperature dependence and $\chi(T)$ approaches a finite value. For the case $S_2 > S_1$, we have finite magnetization $M_f = \frac{S_2-S_1}{2}$ at zero temperature and vanishing magnetic field $(T = 0, h = 0^+)$ in agreement with [18]. In the other limit $(T = 0^+, h = 0)$, we have zero magnetization. This is compatible with the fact that at low temperature and zero magnetic field $\chi(T)$ shows divergent behaviour. For finite (even small) magnetic field the system becomes polarized presenting finite magnetization associated with a drop of $\chi(T)$. In the last case, $S_1 > S_2$, the system behaves as an antiferromagnet. It has zero magnetization in both limits $(T = 0, h = 0^+)$ and $(T = 0^+, h = 0)$ in accordance with [17].

For the cases $S_2 > S_1$ and $S_2 < S_1$, the models present residual entropy. The specific values for this quantity can be extracted from low temperature asymptotic solutions of the non-linear integral equations. The results are given by $S_{res} = \frac{1}{2} \ln [2(S_2 - S_1) + 1]$ and $S_{res} = \frac{1}{2} \ln \left[\frac{\sin \frac{\pi(2S_2+1)}{2S_1+2}}{\sin \frac{\pi}{2S_1+2}} \right]$ for $S_2 > S_1$ and $S_2 < S_1$ respectively. The latter case was considered in [17] for $(S_1 = 1, S_2 = 1/2)$ using the TBA approach. There, however, the exact value of the residual entropy was left open due to limitations of their method.

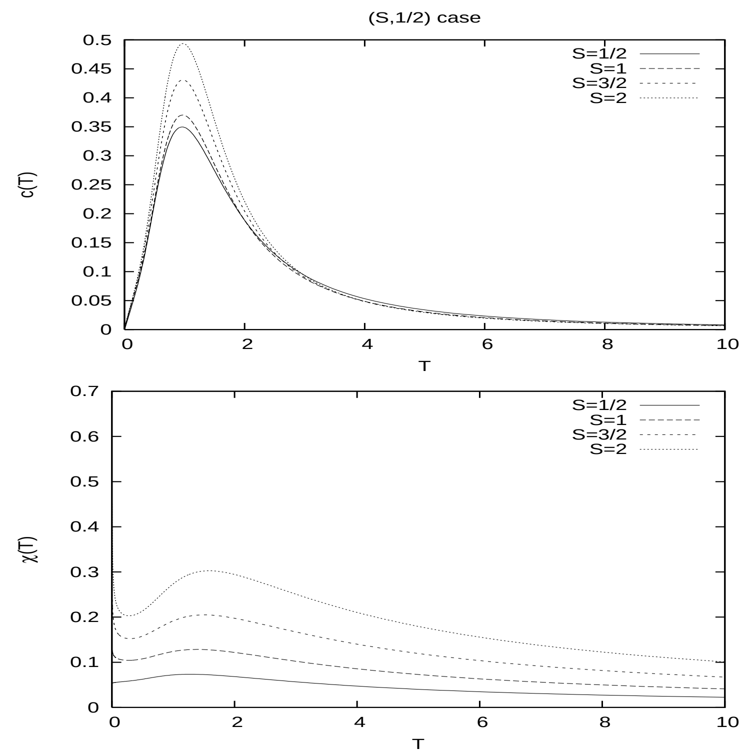

Figure 3: Specific heat $c(T)$ and $\chi(T)$ magnetic susceptibility versus temperature T for $S_1 = S = 1/2, 1, 3/2, 2$ and $S_2 = 1/2$.

6 Thermal current

In this section, we are interested in the thermal Drude weight $D_{th}(T)$ at finite temperature. We restrict ourselves to the case $S_1 = S_2$, where the thermal current is related to the second conserved charge (5) of the transfer matrix.

Specifically, we consider the local conservation of energy in terms of a continuity equation. This relates the time derivative of the local Hamiltonian H_{ii+1} to the divergence of the thermal current j^E, $\dot{H} = -\nabla j^E$. Here, the

local term H_{ii+1} stands for

$$H_{ii+1} = P_{i,i+1}\frac{\partial}{\partial\lambda}\mathcal{L}^{(S_1,S_1)}_{i,i+1}(\lambda)\Big|_{\lambda=0}, \quad \mathcal{H} = \sum_{i=1}^{L} H_{ii+1}. \tag{76}$$

As the time derivative leads to the commutator with the Hamiltonian, we obtain

$$\dot{H}_{i,i+1} = \mathrm{i}\,[\mathcal{H}, H_{i,i+1}(t)] = -\mathrm{i}\left(j^E_{i+1}(t) - j^E_i(t)\right), \tag{77}$$

where the local energy current j^E_i is given by

$$j^E_i = \mathrm{i}\,[H_{i-1i}, H_{ii+1}]\,, \tag{78}$$

and the total thermal current is $\mathcal{J}_E = \sum_{i=1}^{L} j^E_i$.

On the other hand, just by comparing the expression for $\mathcal{J}_E$ and the second logarithmic derivative of the transfer matrix $\mathcal{J}^{(2)}$, we obtain

$$\mathcal{J}_E = \mathcal{J}^{(2)} + \mathrm{i}\frac{L}{2}\frac{\partial^2}{\partial\lambda^2}\zeta_{S_1,S_1}(\lambda)\Big|_{\lambda=0}. \tag{79}$$

The transport coefficients are determined from the Kubo formula [27] in terms of the expectation value of the thermal current $\mathcal{J}_E$, such that [28, 29]

$$D_{th}(T) = \beta^2\left\langle \mathcal{J}_E^2\right\rangle. \tag{80}$$

In order to calculate the expectation value $\langle\mathcal{J}_E^2\rangle$, we introduce a new partition function $\bar{Z}$ as,

$$\bar{Z} = \mathrm{Tr}\left[\exp\left(-\beta\mathcal{H} - \lambda_n\mathcal{J}^{(n)}\right)\right]. \tag{81}$$

In this way, we obtain the expectation values of $\mathcal{J}^{(2)}$ through the logarithmic derivative of $\bar{Z}$,

$$\left(\frac{\partial}{\partial\lambda_2}\right)^2 \ln\bar{Z}\Big|_{\lambda_2=0} = \left\langle\mathcal{J}_E^2\right\rangle, \tag{82}$$

where we used the fact that the expectation value of the thermal current in thermodynamical equilibrium is zero $\langle \mathcal{J}_E \rangle = 0$.

To compute the partition function $\bar{Z}$, we consider the procedure developed in [29]. We rewrite the partition function $\bar{Z}$ in terms of the row-to-row transfer matrix such that

$$\begin{aligned} \bar{Z} &= \lim_{N\to\infty} \mathrm{Tr}\left[\exp\left(T(u_1)\dots T(u_N)T(0)^{-N}\right)\right], \\ &= \mathrm{Tr}\left[\exp\left(\lim_{N\to\infty}\sum_{l=1}^{N}\{\ln T(u_l) - \ln T(0)\}\right)\right]. \end{aligned} \tag{83}$$

The numbers $u_1, \dots, u_N$ are chosen in such a way that the following relation is satisfied,

$$\lim_{N\to\infty}\sum_{l=1}^{N}\{\ln T(u_l) - \ln T(0)\} = -\beta \frac{\partial}{\partial x}\ln T(x)\Big|_{x=0} + \lambda_n \mathrm{i}^{n-1}\frac{\partial^n}{\partial x^n}\ln T(x)\Big|_{x=0}. \tag{84}$$

We can proceed analogously to section 2 and introduce a quantum transfer matrix associated to the partition function $\bar{Z}$. Instead of the staggered vertex model with alternation in vertical direction between $T(-\tau)$ and $\overline{T}(-\tau)$, we have now N different terms of the form $T(0)^{-1}T(u_l)$ for $l = 1, \dots, N$. As $T(0)^{-1} = \overline{T}(0)/\mathcal{N}$, we can write $T(0)^{-1} = [(2S_1)!]^{-2L}T(-\rho)$. So, we have the alternation of $T(-\rho)$ and $T(u_l)$ which is a special case of the previous sections.

Therefore, we can proceed along the same lines as before which is equivalent to substitute $\phi_+(x) \to \prod_{l=1}^{N}\phi_l(x)$ and $\phi_-(x) \to \prod_{l=1}^{N}\phi_0(x)$ where $\phi_l(x) = x - \mathrm{i}u_l$ and $\phi_0(x) = x$.

In this way, the partition function can be written in the thermodynamical

limit in terms of the largest eigenvalue,

$$\lim_{L\to\infty}\frac{1}{L}\ln\bar{Z}=\ln\Lambda(0), \tag{85}$$

which is written as

$$\ln\Lambda(0)=(-\beta+\lambda_n\frac{\partial^{n-1}}{\partial x^{n-1}})\mathcal{E}(x)\Big|_{x=0}+\left(K*\ln B\bar{B}\right)(0), \tag{86}$$

where $\mathcal{E}(x)=\epsilon^{(S_1,S_1)}(x)$.

The auxiliary functions B and $\bar{B}$ satisfy the following set of non-linear integral equations

$$\begin{pmatrix}\ln y^{(\frac{1}{2})}(x)\\ \vdots\\ \ln y^{(S_1-\frac{1}{2})}(x)\\ \ln b(x)\\ \ln\bar{b}(x)\end{pmatrix}=\begin{pmatrix}0\\ \vdots\\ 0\\ (-\beta+\lambda_n\frac{\partial^{n-1}}{\partial x^{n-1}})d(x)\\ (-\beta+\lambda_n\frac{\partial^{n-1}}{\partial x^{n-1}})d(x)\end{pmatrix}+\mathcal{K}*\begin{pmatrix}\ln Y^{(\frac{1}{2})}(x)\\ \vdots\\ \ln Y^{(S_1-\frac{1}{2})}(x)\\ \ln B(x)\\ \ln\bar{B}(x)\end{pmatrix}. \tag{87}$$

Therefore, the thermal Drude weight is given by,

$$D_{th}(T)=\beta^2\left\langle{\mathcal{J}^{(2)}}^2\right\rangle=\beta^2\left(\frac{\partial}{\partial\lambda_2}\right)^2\ln\Lambda(0)\Big|_{\lambda_2=0}. \tag{88}$$

In Figure 4, we show the thermal Drude weight as function of the temperature for $S_1=S_2=S$. It exhibits a linear behaviour at low temperatures and is proportional to the central charge $c=\frac{3S}{S+1}$. This is in agreement with the spin-1/2 case [29].

Before closing this section, we would like to mention that in the general case (S_1,S_2) the thermal current does not look like a conserved current. In this case, we cannot provide exact results for the Drude weight. Nevertheless, we are able to provide an exact description of the second logarithmic

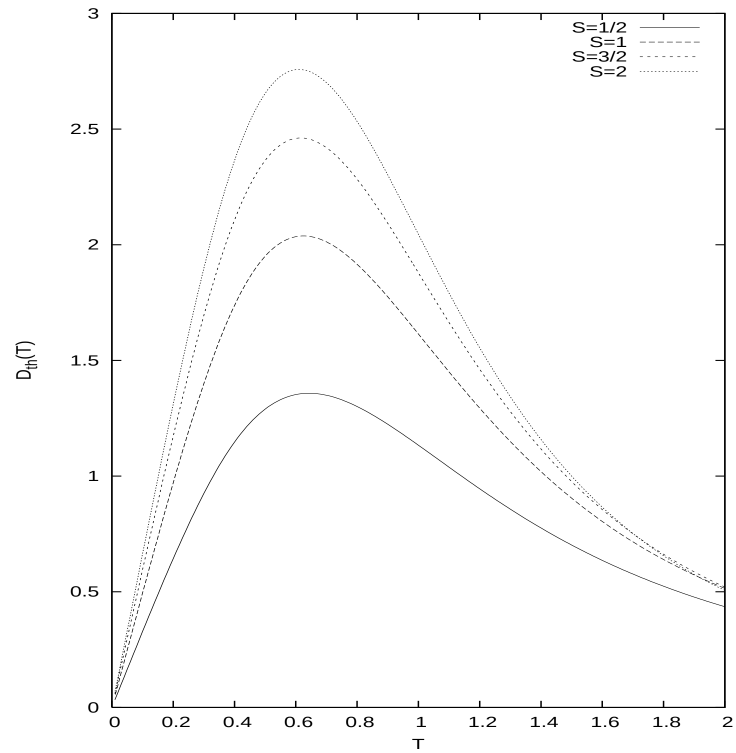

Figure 4: Thermal Drude weight $D_{th}(T)$ as function of temperature for $S = 1/2, 1, 3/2, 2$.

derivative of the transfer matrix. However, the physical interpretation of this quantity has eluded us so far.

7 Conclusion

In this paper we managed to construct the quantum transfer matrix for the case of non-isomorphic auxiliary and quantum spaces of interacting spins. We considered explicitly the generic (S_1, S_2) case of alternating spin chains

and obtained a finite set of non-linear integral equations. These equations were solved numerically for the cases $S_1 < S_2$ and $S_1 \geq S_2$. In this way, we obtained the specific heat and the magnetic susceptibility as functions of temperature. For the particular case $S_1 = S_2$, we also provided results for the thermal Drude weight at finite temperature.

The system behaves antiferromagnetically for $S_1 \geq S_2$ and presents finite magnetization in the remaining case $S_1 < S_2$. Interestingly, for all $S_1 \neq S_2$ we have residual entropy at zero temperature which we were able to evaluate exactly. Recently, systems with finite entropy at $T = 0$ attracted interest regarding efficient cooling procedures [31].

We expect that our results may be interesting for the study of generic mixed spin chains [30]. Another interesting issue deserving investigation is the physical interpretation of the second conserved charge for the generic case (S_1, S_2) and its implications on transport properties.

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